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Quantum Surface of Section Method: Demonstration of semiclassical Berry-Robnik energy level spacing distribution in a generic 2-dim Hamiltonian system

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Abstract The recently developed [12, 14, 24, 15] *quantum surface of section method* is applied to a search for extremely high-lying energy levels in a simple but generic Hamiltonian system between integrability and chaos, namely the *semiseparable 2-dim oscillator*. Using the stretch of 13,445 consecutive levels with the sequential number around $1.8 \cdot 10^7$ (eighteen million) we have clearly demonstrated the validity of the semiclassical Berry-Robnik [3] level spacing distribution while at 1000 times smaller sequential quantum numbers we find the very persistent quasi universal phenomenon of power-law level repulsion [19, 21] which is globally very well described by the Brody distribution.

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The study of energy level statistics of generic quantum Hamiltonian systems whose classical dynamics is between integrability and full chaos persists to be a challenging problem [19, 20, 21]. Until very recently there were incompatible results concerning the so called *level spacing distribution* $P(S)$ where $P(S)dS$ is a probability that a randomly chosen spacing between two adjacent energy levels lies between $S-dS/2$ and $S+dS/2$. Berry and Robnik [3] derived the semiclassical level spacing distribution $P^{\rm BR}(S)$ assuming the *principle of uniform semiclassical condensation* [2, 23, 16, 11, 21] of eigenstates onto classical invariant components (which can be either regular – tori or irregular – chaotic) and the statistical independence of the level subsequences belonging to various disjoint classical invariant components. (Regular levels associated with quantized invariant tori may be merged together giving the well known Poisson distribution $P_{\rm Poisson}(S)=e^{-S}$.) Using the factorization of gap distributions $E(S)=\int_S^\infty d\sigma(\sigma-S)P(S)$ upon statistically independent superposition of spectra one may write

$$E^{\rm BR}_{\rho_1}(S) = E^{\rm Poisson}(\rho_1 S) E^{\rm GOE}(\rho_2 S) \tag{1}$$

for the simplest case of only one chaotic component with relative measure ρ_2 and regular components with total relative measure $\rho_1=1-\rho_2$. The Berry-Robnik distribution does not exhibit *level repulsion*, since $P^{\rm BR}_{\rho_1}(0)=1-\rho_2^2\neq 0$. On the other hand there has been a vast amount of phenomenological evidence [21] in favour of the so called *fractional power law level repulsion* which is globally very well described by the Brody [6] distribution

$$P^B_\beta(S) = aS^\beta \exp(-bS^{\beta+1}), \quad a=(\beta+1)b,\ b=[\Gamma(1+(\beta+1)^{-1})]^{\beta+1} \tag{2}$$

or the more sophisticated Izrailev [10] distribution which are characterized by the noninteger exponent β, $P(S\to 0)\propto S^\beta$. Numerical spectra which contain even up to several ten thousands energy levels of quantum Hamiltonian systems with mixed classical dynamics typically still exhibit the phenomenon of fractional level repulsion, with statistically significant global fit by the Brody distribution. In such cases there was a persisting puzzle how the level spacing distribution converges to the semiclassical Berry-Robnik distribution as one increases the sequential quantum number or decreases the value of effective $\hbar$. However, recently we have succeeded to demonstrate the ultimate semiclassical Berry-Robnik level spacing distribution in a rather abstract 1-dim time-dependent dynamical system, namely the standard map on a torus, and showed the smooth transition from Brody-like to Berry-Robnik distribution as $\hbar$ decreases [20, 21] (see also [13]). The transition was excellently described by two parameter (ρ_1,β) Berry-Robnik-Brody model in which we substitute the GOE model for the chaotic part $E^{\rm GOE}(\rho_2 S)$ in Berry-Robnik formula (1) by the Brody model $E^{\rm B}_\beta(\rho_2 S)$ with some exponent β. The major goal of this letter is to demonstrate this scenario in a *generic 2-dim autonomous Hamiltonian system.*

Another goal of this letter is to demonstrate the practical power of the recently developed *quantum surface of section method* [12, 14, 24] (which has been motivated by the semiclassical version developed in [4] and extensively numerically investigated

in [8]) and whose most thorough and complete presentation so far is given in [15]. We shall use the reactance matrix formulation of the quantization condition which has practical advantages over the scattering matrix formulation in the case of semiseparable systems ([15], section 2.7). Here we give a brief and hence rather heuristic description of the method for the quantum Hamiltonians $\hat{H}$ in 2-dimensional configuration space (CS) with coordinates (x, y) where the line $y = 0$ represents the *configurational surface of section* (CSOS) while we use Dirichlet boundary conditions on the boundary lines $y = b_\uparrow > 0$ and $y = -b_\downarrow < 0$. Let $\Psi_{\sigma n}(x, y, E)$ be the solutions of the Schrödinger equation $\hat{H}\Psi_{\sigma n}(x, y, E) = E\Psi_{\sigma n}(x, y, E)$ on the upper $(y > 0, \sigma = \uparrow = +)$ / lower $(y < 0, \sigma = \downarrow = -)$ side of CS which satisfy the boundary conditions $\Psi_{\sigma n}(x, 0, E) = u_n(x), \quad \Psi_{\sigma n}(x, \sigma b_\sigma, E) = 0$, and $u_n(x)$ is some complete set of functions for the *small* Hilbert space of L^2 functions over 1-dim CSOS, e.g the eigenfunction of the *reduced* Hamiltonian $\check{H}' = \hat{H}|_{y=0}$, $\check{H}'u_n(x) = E'_n u_n(x)$. The full eigenfunction $\Psi(x, y, E)$ of $\hat{H}$ can be expanded in terms of partial eigenfunctions $\Psi_{\sigma n}(x, y, E)$ on both sides as $\Psi(x, y, E) = \sum_n c_{\sigma n}|k_n(E)|^{-1/2}\Psi_{\sigma n}(x, y, E)$, where $\sigma = \mathrm{sign}(y)$ while the square roots of the *wavenumbers* $k_n = \hbar^{-1}\sqrt{2m(E - E'_n)}$ provide a useful normalization. In order that $\Psi(x, y, E)$ would be a nontrivial eigenfunction on the entire CS it should be continuously differentiable on CSOS (at $y = 0$). Using the completeness of the set $u_n(x)$ the requirement for continuity gives $c_{\uparrow n} = c_{\downarrow n}$, whereas requiring continuity of the normal derivative yields the singularity condition for the *real symmetric reactance matrix* $\tilde{\mathbf{R}} = \tilde{\mathbf{R}}_\uparrow + \tilde{\mathbf{R}}_\downarrow$,

$$\tilde{\mathbf{R}}_{\sigma n l}(E) = \sigma|k_n(E)k_l(E)|^{-1/2}\int dx \Psi_{\sigma n}(x, 0)\partial_y \Psi_{\sigma l}(x, 0), \tag{3}$$

$$\det \tilde{\mathbf{R}}(E) = 0. \tag{4}$$

This equation is equivalent to the more physical but numerically less effective (due to complex non-symmetric arithmetic) quantization condition $\det(1 - \mathbf{T}_\downarrow(E)\mathbf{T}_\uparrow(E)) = 0$ [12, 14, 24, 15] in terms of generalized (*non-unitary*) scattering matrices $\mathbf{T}_\sigma(E)$ of the two scattering problems (obtained by cutting one half of the CS along CSOS off and attaching the waveguide (flat in the y-direction) instead) which have a finite number N_o of propagating – open, and infinitely many evanescent – closed modes $e^{\pm ik_n(E)y}u_n(x)$, for $k_n^2(E) > 0$, and $k_n^2(E) < 0$, respectively. The scattering matrices are related to (*non-real*) reactance matrices, by $\mathbf{T}_\sigma = (1 + i\mathbf{R}_\sigma)(1 - i\mathbf{R}_\sigma)^{-1}$, where the latter are made real by a simple diagonal transformation $\tilde{\mathbf{R}}_\sigma = \mathbf{D}\mathbf{R}_\sigma\mathbf{D}$, where $\mathbf{D} = \mathrm{diag}(1, 1 \ldots N_o \; times \ldots 1, \sqrt{i}, \sqrt{i} \ldots)$.

We have applied this method to a semiseparable system which is separable above/below CSOS but not separable on the whole CS, namely to 2-dim semiseparable oscillator (SSO) with the Hamiltonian

$$\hat{H} = -\tfrac{1}{2}\hbar^2(\partial_y^2 + \partial_x^2) + \tfrac{1}{2}(x - \tfrac{1}{2}\mathrm{sign}(y)a)^2, \quad -b_\downarrow \le y \le b_\uparrow, \tag{5}$$

with the parameters $a, b_\sigma, \hbar$. SSO has a scaling symmetry $(a, b_\sigma, \hbar, E) \to (\alpha a, \alpha b_\sigma, \alpha^2\hbar, \alpha^2 E)$. The reduced Hamiltonian is just a simple 1-dim harmonic oscillator $-\frac{1}{2}\hbar^2\partial_x^2 + \frac{1}{2}x^2$ with eigenfunctions $u_n(x) = (\sqrt{\pi\hbar}2^n n!)^{-1/2}\exp(-x^2/2\hbar)H_n(x/\sqrt{\hbar})$ and eigenenergies $E'_n = (n+\frac{1}{2})\hbar$ determining the wavenumbers $k_n(E) = \hbar^{-1}\sqrt{2E - (2n+1)\hbar}$, $n =$

$0, 1 \ldots$ It is easy to derive an explicit expression for the reactance matrices for SSO

$$\tilde{\mathbf{R}}_\uparrow(E) = \mathbf{J}(E)\mathbf{O}\mathbf{C}_\uparrow(E)\mathbf{O}^T\mathbf{J}(E), \quad \tilde{\mathbf{R}}_\downarrow(E) = \mathbf{J}(E)\mathbf{O}^T\mathbf{C}_\downarrow(E)\mathbf{O}\mathbf{J}(E), \tag{6}$$

where $\mathbf{J}(E), \mathbf{C}_\sigma(E)$ are *real diagonal matrices*

$$\mathbf{J}_{nl}(E) = \delta_{nl}|k_n(E)|^{-1/2}, \quad \mathbf{C}_{\sigma nl}(E) = \delta_{nl}k_n(E)\cot(k_n(E)b_\sigma), \tag{7}$$

and $\mathbf{O}$ is *real orthogonal shift matrix*

$$\mathbf{O}_{nl} = \int dx u_n(x) u_l(x + \tfrac{1}{2}a) \tag{8}$$

whose matrix elements can be calculated via *numerically stable* symmetric recursion

$$\begin{aligned}
\mathbf{O}_{n,0} &= \frac{1}{\sqrt{n!}} \exp\left(-\frac{a^2}{16\hbar}\right), \quad \mathbf{O}_{0,l} = \frac{(-1)^l}{\sqrt{l!}} \exp\left(-\frac{a^2}{16\hbar}\right), \\
\mathbf{O}_{n,l} &= \frac{1}{2}\left(\sqrt{\frac{n}{l}} + \sqrt{\frac{l}{n}}\right)\mathbf{O}_{n-1,l-1} + \frac{a}{\sqrt{32\hbar n}}\mathbf{O}_{n-1,l} - \frac{a}{\sqrt{32\hbar l}}\mathbf{O}_{n,l-1}.
\end{aligned}$$

It is important how to truncate these infinitely dimensional matrices for the numerical calculation. One has to consider all the $N_o = \mathrm{round}(E/\hbar)$ open modes plus as many N_c closed modes so that the numerical results (roots of eq. (4)) converge. I have used semiclassical arguments (the SOS (x, p_x) phase space supports of coherent state representation of the states $u_n(x), n = 1, \ldots, N_o + N_c$ should cover the supports of the states $u_l(x + \frac{1}{2}a), l = 1, \ldots, N_o$) to estimate the minimal number of closed modes

$$N_c \approx \left(\frac{2a}{\sqrt{2E}} + \frac{a^2}{2E}\right) N_o. \tag{9}$$

Dimension of matrices $N = N_o + N_c$ is thus usually (for small a) only little larger than the number of open modes N_o.

It is also very important to stress that the shift matrix and therefore also the reactance matrices are *effectively banded*. I have obtained semiclassical formula for their bandwidths using overlap condition for the coherent state representation of the SOS-states $u_n(x)$ and $u_l(x + \frac{1}{2}a)$

$$\mathrm{bandwidth}(\mathbf{R}_\sigma) = 2\,\mathrm{bandwidth}(\mathbf{O}) \approx \frac{a}{\hbar}\sqrt{2E}. \tag{10}$$

Note that the function $f(E) = \det \tilde{\mathbf{R}}(E)$ has singularities (poles) at the points E where for some n, $k_n(E)b_\sigma$ is a multiple of π. But between the two successive poles $f(E)$ is smooth (even analytic) real function of real energy E. I have devised an algorithm for calculation of almost all levels — zeros of $f(E)$ within a given interval $[E_i, E_f]$ which needs to evaluate $f(E)$ only about 25 times per mean level spacing while it typically misses less than 0.5% of all levels. The control over missed levels is in general very difficult problem. The number of all energy levels below a given energy E, $\mathcal{N}(E)$ can be estimated by means of the Thomas-Fermi rule

$$\mathcal{N}(E) \approx \mathcal{N}^{\mathrm{TF}}(E) = \frac{b_\uparrow + b_\downarrow}{3\pi\hbar^2}(2E)^{3/2} = \mathcal{O}(N^2). \tag{11}$$

But this formula is generally not very helpful even if next semiclassical corrections are negligible since the fluctuation of the number of levels in an interval $[E_i, E_f]$ is proportional to $\sqrt{\mathcal{N}(E_f) - \mathcal{N}(E_i)}$ except in the extreme case of fully chaotic systems where the spectra are much stiffer and the fluctuation is proportional to $\log[\mathcal{N}(E_f) - \mathcal{N}(E_i)]$ so that Thomas-Fermi rule can be used to detect even single missing level [5, 1].

We have chosen the following values of the parameters for our numerical demonstration $a = 0.03, b_\uparrow = 5.0, b_\downarrow = 10.0, E = 0.5$ while for quantal calculations we take energy to be in narrow interval around $E = 0.5$. For illustration we plot the classical SOS $(x, p_x, y = 0)$ in figure 1. There is only one dominating chaotic component with relative measure $\rho_2 = 0.709 \pm 0.001$ and the regular region still with some very small chaotic components with the complementary total relative measure $\rho_1 = 1 - \rho_2 = 0.291 \pm 0.001$. For the quantal calculations we have chosen two different values of $\hbar = 0.01$ and $\hbar = 0.0003$ which correspond to sequential numbers $\mathcal{N} \approx 16\,000$ and $\mathcal{N} \approx 17\,684\,000$, respectively.

In the first case ($\hbar = 0.01, \mathcal{N} \approx 1.6 \cdot 10^4$) we have calculated 14 231 levels in the interval $0.35 < E < 0.65$. We have performed a χ^2 test and obtained *statistically significant* fit of $P(S)$ by the Brody distribution with $\beta = 0.142, \chi^2_{\rm B} = 5320$ and *nonsignificant* Berry-Robnik fit with $\rho_1 = 0.548, \chi^2_{\rm BR} = 130\,000$ (see figure 2). In order to present most detailed information we plot cumulative level spacing distribution $W(S) = \int_0^S d\sigma P(\sigma)$ and deviation of numerical $U-$function [19] $U(W(S)) = (2/\pi)\arccos(\sqrt{1 - W(S)})$ from the best fit Berry-Robnik U-function $U(W^{\rm BR}(S))$ versus $W(S)$ which has a nice property that the estimated statistical error $\delta U = 1/\pi\sqrt{N}$ and the density of numerical points along abscissa are constant. In spite of the already very high sequential number this is still an example of the so-called near-semiclassical regime characterized by the fractional power law level repulsion.

In the second case ($\hbar = 0.0003, \mathcal{N} \approx 1.8 \cdot 10^7$) we have calculated 13 445 levels on the interval $0.49985 < E < 0.500105$ and found *significant* fit by the semiclassical Berry-Robnik formula (see figure 3) with the *correct* value of regular volume $\rho_1 = 0.286 \pm 0.005, \chi^2_{\rm BR} = 12\,150$ while Brody fit becomes highly nonsignificant, $\beta = 0.367, \chi^2_{\rm B} = 249\,000$. Thus we have demonstrated the so-called far semiclassical regime with the quantum value of ρ_1 which excellently agrees with the classical regular volume (the small deviation is within error bars). Fit to combined Berry-Robnik-Brody model *does not* not significantly improve $\chi^2 = 11\,950$ while it substitutes GOE model for the chaotic part by the Brody model with $\beta \approx 0.85$.

Large square root number fluctuations prevent to determine the number of missed levels by using Thomas-Fermi rule (although higher order semiclassical corrections are negligible in this regime). One can compare the number of levels $\mathcal{N}(E)$ with the number of levels $\mathcal{N}_0(E)$ or $\mathcal{N}_\infty(E)$ for the two nearby integrable – separable cases (with the same b_σ but with $a = 0$ (single box limit) or $a \to \infty$ (two box limit), respectively) since the leading order semiclassics (Thomas-Fermi rule) does not depend upon defect a. $\mathcal{N}_0(E)$ and $\mathcal{N}_\infty(E)$ can be easily calculated numerically and

large scale fluctuations of $\mathcal{N}(E) - \mathcal{N}_{0,\infty}(E)$ turn out to be much smaller than the fluctuations of $\mathcal{N}(E) - \mathcal{N}^{\mathrm{TF}}(E)$ suggesting that we have missed *less* than 20 levels out of 14 231 at $\hbar = 0.01$ (figure 2) and 40 - 80 levels out of 13 445 at $\hbar = 0.0003$ (figure 3). Note that in the first case ($\hbar = 0.01$) there was much less almost degenerate pairs of levels (and therefore missed levels) due to the level repulsion.

In conclusion I should emphasize that the present work presents clear demonstration of the semiclassical Berry-Robnik level spacing distribution in a generic 2-dim autonomous Hamiltonian system between integrability and chaos, i.e. semiseparable oscillator. This would not be possible without application of the quantum surface of section method which enabled us to calculate 13 445 consecutive levels with sequential numbers $\mathcal{N} \approx 1.8 \cdot 10^7$ within a week of Convex 3680 CPU time. For this system, quantum surface of section method requires $\mathcal{O}(a^2\mathcal{N}^{3/2})$ FPO/level. In the forthcoming publications I will [17] discuss in detail the energy spectra, quantum eigenstates, and quantum SOS evolution by the quantum SOS method in the semiseparable oscillator, and [18] apply the quantum SOS method to a more realistic example, namely the diamagnetic Kepler problem [9, 7, 22].

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Figures

Figure 1 Classical surface of section $y = 0$ with coordinates x, p_x of the semiseparable oscillator $a = 0.03, b_\uparrow = 5.0, b_\downarrow = 10.0, E = 0.5$. 250 orbits with 40 000 crossings of SOS each are shown.

Figure 2 Cumulative level spacing distribution $W(S)$ (a) and deviation of its U-function from the best fit Berry-Robnik distribution (b) for 14 231 consecutive levels of SSO at $a = 0.03, b_\uparrow = 5.0, b_\downarrow = 10.0, 0.35 < E < 0.65, \hbar = 0.01$. Thick full curves (a,b) (within $\pm$ one sigma error band (b)) represent numerical data, the thin full curve (a) is best fit Berry-Robnik distribution with $\rho_1 = 0.548$ whereas the dashed curves (a,b) is the best fit Brody distribution with $\beta = 0.142$. The dotted curves (a) represent the limiting Poisson and GOE distributions whereas the dash-dotted curves (b) represent the nearby Berry-Robnik curves with $\rho_1 = 0.548 \pm 0.01, \pm 0.02$.

Figure 3 The same as in figure 2 but now at $\hbar = 0.0003$ for 13 445 levels in the interval $0.49985 < E < 0.500105$ living in the true (far) semiclassical regime (see text). The Berry-Robnik distribution with $\rho 1 = 0.287$ is now statistically significant and for illustration of accuracy of the fitted ρ_1 we provide also Berry-Robnik curves for $\rho_1 = 0.287 \pm 0.01, \pm 0.02$ (dash-dotted curves (b)).